COPY NO. 1

~~NEW YORK UNIVERSITY~~
~~INSTITUTE OF MATHEMATICAL SCIENCES~~
~~LIBRARY~~
~~25 Waverly Place, New York 3, N.Y.~~

IMM-NYU 218
MAY 1955

IMM 218

NEW YORK UNIVERSITY
INSTITUTE OF
MATHEMATICAL SCIENCES

NEW YORK UNIVERSITY
COURANT INSTITUTE - LIBRARY
251 Mercer St. New York, N.Y. 10012

On the Adiabatic Theorem in Quantum Theory

K. O. FRIEDRICHS

PART I.

PREPARED UNDER
CONTRACT NO. DA-30-069-ORD-1258
WITH THE
OFFICE OF ORDNANCE RESEARCH, U. S. ARMY

NEW YORK UNIVERSITY
COURANT INSTITUTE - LIBRARY
251 Mercer St. New York, N.Y. 10012

~~NEW YORK UNIVERSITY~~
~~INSTITUTE OF MATHEMATICAL SCIENCES~~
~~LIBRARY~~
~~25 Waverly Place, New York 3, N.Y.~~

NEW YORK UNIVERSITY
COURANT INSTITUTE - LIBRARY
251 Mercer St. New York, N.Y. 10012

~~NEW YORK UNIVERSITY~~
~~INSTITUTE OF MATHEMATICAL SCIENCES~~
~~LIBRARY~~
~~25 Waverly Place, New York 3, N. Y.~~

IMM-NYU 218
May 1955

ON THE ADIABATIC THEOREM IN QUANTUM THEORY

by

K. O. Friedrichs

PART I.

This paper represents results obtained at the Institute of Mathematical Sciences, New York University, under the sponsorship of Contract DA-30-069-ORD-1258, with the Office of Ordnance Research, U. S. Army.

New York 1955

On the Adiabatic Theorem in Quantum Theory

by

K. O. Friedrichs

Part I

The adiabatic theorem in quantum theory refers to a situation in which the original Hamiltonian of a system is gradually changed into a new Hamiltonian. Roughly speaking, the theorem states that an eigenstate for the original energy goes approximately over into an eigenstate for the new energy if the switch-on of the energy difference is sufficiently slow.

A first treatment of the adiabatic theorem was given by Born [1] in 1926 in the case that the energy operator has a pure point spectrum. Later on Born and Fock [2] supplied rigorous arguments covering also the cases of degenerate spectra.[1] A different approach was given by Kato [7]. An adiabatic theorem in a typical case in which the Hamiltonian has a continuous spectrum was given by Snyder [9]. In the present paper both cases will be dealt with systematically.

To obtain a precise formulation of the adiabatic theorem one must consider a manifold of Hamiltonians which depend on the time t and, in addition, on a parameter τ which measures the degree of "slowness" of the switch-on process. We suppose the transition from the initial into the final Hamiltonian is attained during a time interval $t_0 \leq t \leq t_1$ whose length depends on τ in such a way as to tend to ∞ together

---

[1] The paper by Born and Fock contains a bibliography of work on the adiabatic theorem in the old quantum theory and in classical dynamics.

with τ. The solution of the Schrödinger equation associated with the Hamiltonian clearly depends on the parameter τ and one aims at an asymptotic description of this solution which is valid during the whole time interval $t_o \leq t \leq t_1$ provided τ, and hence $t_1 - t_o$, is sufficiently large.

The first term in the asymptotic expansion of the Schrödinger solution will lead to a "general adiabatic theorem".

It is a consequence of this theorem that every eigenstate of the initial Hamiltonian $\Phi^{(o)}$ goes over into an eigenstate $\Phi^{(1)}$ of the final Hamiltonian. We shall refer to this statement as the "special adiabatic theorem".

Born and Fock, and similarly Kato, give an estimate of the order of magnitude of the deviation of the first term from the exact solution. We shall go further and describe the terms of the asymptotic expansion in the case that the Hamiltonian has a pure non-degenerate point spectrum.

We then can determine - to lowest order - the probability that an eigenstate $\Phi^{(o)}$ of the initial Hamiltonian does not go over into the eigenstate $\Phi^{(1)}$ of the final Hamiltonian; or - as we may say - that the transition is not adiabatic. This probability is of the order $O(\tau^{-2})$.

The second term of the asymptotic expansion derived under the assumption that all eigenvalues of $H(t)$ remain distinct is not valid in the case that two eigenvalues become equal at some time in the interval $t_o < t < t_1$. We shall treat such a

case in Part II of this report. The problem is essentially a turning point problem analogous to that treated by Jeffreys, Kramers, Langer, and others. As a result we find a simple expression of the order $O(\tau^{-1})$, for the probability that the transition is not adiabatic. Actually we shall treat only the case in which the Hilbert space of states is two-dimensional. We believe that the results obtained are typical.

The knowledge that in first approximation an eigenstate of the initial Hamiltonian runs through eigenstates of the time dependent Hamiltonian is not sufficient to determine the first term in the asymptotic expansion of the Schrödinger solution; for, these eigenstates are determined only within a factor of absolute value 1. This factor must be characterized by an appropriate condition. This condition can be given in an "intrinsic" form which depends on the nature of the spectrum of the Hamiltonian. The specific condition which is appropriate for operators with a pure point spectrum was already given by Fock [2]. It is remarkable that the specific condition appropriate for a typical class of operators with continuous spectra is essentially different from Fock's condition; it is closely connected with the radiation condition in the theory of scattering.

The relationship between the adiabatic theorem and the properties of the scattering operator was pointed out by Snyder (see also the report by Moses [13]). We shall explain this relationship and also derive the "principle of the irrelevancy of the adiabatic hypothesis" formulated by Snyder.

Finally, we shall treat[*] a simple problem occurring in the quantum theory of fields, in which the Hamiltonian displays discrete features although it is continuous except for a single point eigenvalue. Fock's condition for discrete spectra is appropriate in this case. That this is so can be verified from the exact solution of the Schrödinger equation, which can be given explicitly.

1. Schrödinger Equation

The Hamiltonians, or "energy operators", at the initial time $t = t_o$ and at the final time t_1 will be denoted by H_o and H_1 respectively. For intervening times t the Hamiltonian is then given as a function[2]

$$H = H(t,\tau) \tag{1.1}$$

of the time t and the slowness parameter τ in such a way that

$$H(t_o(\tau),\tau) = H_o \qquad H(t_1(\tau),\tau) = H, \tag{1.2}$$

where $t_o(\tau)$ and $t_1(\tau)$ are given functions of τ for which

$$t_1(\tau) - t_o(\tau) \longrightarrow \infty \qquad \text{as } \tau \longrightarrow \infty. \tag{1.3}$$

The Schrödinger operator $T = T(t,\tau)$, i.e. the unitary operator which transforms the state of the system at the time

---

[2] See remark I in the appendix.

[*] In Part II to be issued separately.

$t = t_o$ into its Schrödinger state at the time t, is then defined as the solution of the differential equation

$$(1.4) \qquad i \nabla_t T = H(t,\tau)T$$

for which

$$(1.5) \qquad T(t_o,\tau) = 1.$$

(As usual we set $\frac{h}{r} = 1.$) Our aim is to describe $T(t,\tau)$ asymptotically for large values of τ, uniformly for $t_o(\tau) \leq t \leq t_1(\tau)$.

Following Born and Fock we make a simplifying assumption about the nature of the function $H(t,\tau)$. We assume that there is a function H_s of one variable s which reduces to H_o and H_1 for s = 0 and s = 1, such that $H(t,\tau)$ is of the form

$$(1.6) \qquad H(t,\tau) = H_s$$

with

$$(1.6)' \qquad s = (t - t_o)/\tau.$$

The function $t_1(\tau) - t_o(\tau)$ simply reduces to

$$(1.7) \qquad t_1(\tau) - t_o(\tau) = \tau$$

in this case. This assumption about the dependence of the energy on t and τ is not a serious restriction; it is made solely for simplicity.

The differential equation for the Schrödinger operator T can now be written in the form

(1.8) $i\nabla_s T = \tau H_s T$

in which s, instead of t, is taken as independent variable. The initial condition (1.5) for the operator T is

(1.9) $T = 1$ when $s = 0$.

If we want to exhibit the dependence of the operator T on s and the parameter τ we write $T = T_s(\tau)$, indicating dependence on s by a subscript -- as we shall do quite generally.

Our problem now reduces to that of finding an asymptotic expression of the operator $T(\tau)$ which is valid for $0 \leq s \leq 1$ as $\tau \longrightarrow \infty$. Of course, letting the switch-on time τ become infinite means making the switch-on process "infinitely slow".

Instead of restricting the parameter s to the domain $0 \leq s \leq 1$, as we have done, we could also take the domain $0 \leq s < \infty$ without any essential change.

In the subsequent considerations we shall assume that the Schrödinger equation (1.8) possesses a solution $T_s(\tau)$ which has all desired continuity and differentiability properties. Later on we shall indicate how the existence of this solution can be established.

Suppose the Hilbert space of states is finite-dimensional so that the states can be represented by a finite number of components and the operator H_s by a matrix. Since the

Schrödinger equation then appears as a system of ordinary differential equations of first order, the results of the theory of asymptotic expansion of solutions of such equations could be used to establish the adiabatic theorem. In fact, it would seem likely that the methods developed by Birkhoff and others for ordinary differential equations could be adapted to the present problem in Hilbert space. Our treatment of the problem may perhaps be considered a first step in this direction.

2. Spectral Transformation

We must make various assumptions and introduce various notions before we can give an asymptotic description of the operator $T_s(\tau)$. The basic assumption to be made is that the spectra of the operators H_1 and H_0 and, more generally, of the operators H_s and H_0 can be put in a one-to-one correspondence. That does not mean that the operators H_s and H_0 are unitarily equivalent and thus have the same spectra; but it does mean that H_s and H_0 are functions of two operators N_s and N_0 which are unitarily equivalent. For reasons that will become clear, the operators N_s will be termed "label operators". Unitary equivalence of two operators N_s and N_0 means that a unitary operator U_s exists such that

(2.1) $$N_s = U_s N_o U_s^{-1} \quad .$$

The function with the aid of which the operator H_s will be expressed in terms of the operator N_s will be denoted by $h_s(n)$, so that we may formulate our assumption by saying that unitary operators U_s with $U_o = 1$ and functions $h_s(n)$ exist such that

(2.2) $$H_s = h_s(N_s) \ , \qquad H_o = h_o(N_o) \quad ,$$

when N_s is given by (2.1) .

In order to explain the significance of the label operators N_s , let us consider the case in which the operators H_s have pure point spectra consisting of eigenvalues $h_s^{(1)}$, $h_s^{(2)}$, ... associated with a sequence of eigenstates $\underline{\Phi}_s^{(1)}$, $\underline{\Phi}_s^{(2)}$, ... If the state $\underline{\Phi}$ is given as a series

(2.3) $$\underline{\Phi} = \sum_n c_s^{(n)} \underline{\Phi}_s^{(n)} \quad ,$$

application of the operator H_s can be described by

(2.4) $$H_s \underline{\Phi} = \sum_n h_s^{(n)} c_s^{(n)} \underline{\Phi}_s^{(n)} \quad .$$

As operator N_s we now may choose the operator which is described by

$$(2.5) \qquad N_s \underline{\Phi} = \sum_n n c_s^{(n)} \underline{\Phi}_s^{(n)} \quad .$$

The spectrum of the operator N_s consists of the numbers $n = 1, 2, 3, \ldots$. Since this spectrum is independent of s, a unitary operator U_s such that (2.1) holds exists. The operator which transforms the state

$$(2.6) \qquad \underline{\Phi} = \sum_n c_o^{(n)} \underline{\Phi}_o^{(n)}$$

into the state

$$(2.7) \qquad U_s \underline{\Phi} = \sum_n c_o^{(n)} \underline{\Phi}_s^{(n)}$$

is such an operator U_s . Similarly, U_s^{-1} transforms the state $\underline{\Phi}$, as given by (2.5), into the state

$$(2.8) \qquad U_s^{-1} \underline{\Phi} = \sum_n c_s^{(n)} \underline{\Phi}_o^{(n)} \quad .$$

Relation (2.1) is immediately verified. The function $h_s(n)$ which enters the description (2.2) of the operator H_s is simply given by

$$(2.9) \qquad h_s(n) = h_s^{(n)} \quad ;$$

this function is defined only for positive integers of the variable n, i.e. on the spectrum of the operator N_s ; and that is perfectly sufficient.

A possible interpretation of the label operator in case the operators H_s have continuous spectra will be described later on, in Section 9.

We shall employ a slight generalization of the notion of label operator as given. We shall denote by N a finite number of operators, $N = \left\{ N^{(1)}, \ldots, N^{(\nu)} \right\}$, all satisfying relation (2.1). The letter n then stands for the corresponding system of possible eigenvalues, $n = \left\{ n^{(1)}, \ldots, n^{(\nu)} \right\}$ This system of numbers will be interpreted as a "point" in a ν-dimensional space, the "n-space". However, we shall continue to speak of "one" operator N . Relations (2.1) and (2.2) are then abbreviations for the raltions

$$(2.1') \qquad \begin{aligned} N_s^{(1)} &= U_s N_o^{(1)} U_s^{-1} \quad , \\ &\ldots \\ N_s^{(\nu)} &= U_s N_o^{(\nu)} U_s^{-1} \end{aligned}$$

and

$$(2.2') \qquad \begin{aligned} H_s &= h_s(N_s^{(1)}, \ldots, N_s^{(\nu)}) \ , \\ H_o &= h_o(N_o^{(1)}, \ldots, N_o^{(\nu)}) \ . \end{aligned}$$

An important property of the operator U_s is that relation

$$(2.10) \qquad b(N_s) = U_s b(N_o) U_s^{-1}$$

holds whenever b(n) is a bounded piecewise continuous function of n, as follows from relation (2.1). The condition here imposed on the function b(n) is stronger than necessary. We do not specify an appropriate more general class of functions b(n); but we require that the function $h_s(n)$, which occurs in the definition (2.2) of the Hamiltonian H_s, is such that the relation

$$(2.11) \qquad H_s = h_s(N_s) = U_s h_s(N_o) U_s^{-1} \quad ,$$

holds[3]. The operator $h_s(N_o)$, which will be used frequently in the following, has evidently the same spectrum as H_s; of course, this operator should not be confused with the operator $H_o = h_o(N_o)$.

The significance of the unitary operator U_s is that it gives the spectral transformation for the operator N_s. In

---

[3] Born and Fock employ a transformation V_s which transforms the operator $H_s^{(o)}$, (i.e. H_s in our notation), into a diagonal matrix $V^* H_s^{(o)} V_s$. (We have supplied the subscript s ommitted by them). Our operator U_s -- or rather the special operator $U_s = W_s$ introduced later on -- can be expressed as

$$W_s = V_s V_o^* \quad .$$

order to explain what we mean by this, we must employ an appropriate generalization of the notion of eigenstate associated with a point eigenvalue. Although one could employ the notion of improper eigenstate associated with a point of the continuous spectrum we prefer to introduce the notion of eigenstate associated with a set of eigenvalues. Specifically, we introduce the notion of eigenstate for the operator N_s associated with a set $\mathcal{M}$ in the n-space. By this we mean any state $\underline{\Phi}^{\mathcal{M}} \neq 0$ for which the relation

$$b_{\mathcal{M}}(N_s)\underline{\Phi}^{\mathcal{M}} = 0 \tag{2.12}$$

holds whenever $b_{\mathcal{M}}(n)$ is a bounded, piecewise continuous function which vanishes if the argument n lies in the set $\mathcal{M}$. The set $\mathcal{M}$ will then be called "eigenset" for the state $\underline{\Phi}^{\mathcal{M}}$. Using these notions we define: a unitary operator U_s gives the spectral transformation for the operator N_s if every eigenstate $\underline{\Phi}_o^{\mathcal{M}}$ for the operator N_o with the eigenset $\mathcal{M}$ is transformed by U_s into an eigenstate

$$\underline{\Phi}_s^{\mathcal{M}} = U_s\underline{\Phi}_o^{\mathcal{M}} \tag{2.13}$$

for the operator N_s with the same eigenset $\mathcal{M}$.

The statement made above, that an operator U_s which satisfies relation (2.1) gives the spectral transformation of

the operator N_s , is now seen to mean that the relation

$$(2.14)_o \qquad b_{\mathcal{M}}(N_o)\Phi_o^{\mathcal{M}} = 0$$

entails the relation

$$(2.14)_s \qquad b_{\mathcal{M}}(N_s)\Phi_s^{\mathcal{M}} = 0 .$$

This statement is an immediate consequence of relation

$$b_{\mathcal{M}}(N_s)\Phi_s^{\mathcal{M}} = U_s b_{\mathcal{M}}(N_o)U_s^{-1}U_s\Phi_o^{\mathcal{M}} = U_s b_{\mathcal{M}}(N_o)\Phi_o^{\mathcal{M}} = 0 ,$$

which follows from relation (2.11) for $b(n) = b_{\mathcal{M}}(n)$.

The state $\Phi_s^{\mathcal{M}}$ may also be termed eigenstate for the operator $H_s = h_s(N_s)$; but the corresponding "eigenset" is the image of the set $\mathcal{M}$ under the mapping $h = h_s(n)$. The corresponding eigensets of the operators H_s and H_o are thus in general different.

Let us consider the special case in which the set $\mathcal{M}$ consists of just one point m . In this case we may choose $b_{\mathcal{M}}(n) = n - m$. Setting $\Phi_s = \Phi_s^m$, relation (2.12) reduces to

$$(2.15) \qquad (N_s - m)\Phi_s^m = 0 .$$

In this case then the state Φ_s^m is an ordinary eigenstate for

the operator N_s with the point-eigenvalue m. Clearly, the state Φ_s^m is also eigenstate for the operator $H = h_s(N_s)$ with the eigenvalue $h_s(m)$. Thus we see that the unitary operator U_s transforms an ordinary eigenstate Φ_s^m for the operators N_o and H_o into ordinary eigenstates for the operators N_s and H_s.

Our asymptotic description of the Schrödinger operator $T_s(\tau)$ will imply the statement that this operator approaches -- in a sense to be formulated -- a particular one among the spectral transformations U_s as τ approaches infinity. This statement will be called the "general adiabatic theorem." The remarks made in the preceding paragraph make it clear that the "special adiabatic theorem" indicated at the beginning of this note is an immediate consequence of this general adiabatic theorem.

It is important to note that the unitary operator U_s is not uniquely determined by condition (2.1). If U_s^a is one such unitary operator, every operator of the form

$$U_s = U_s^a \exp \left\{ i\theta_s(N_o) \right\} , \tag{2.16}$$

involving any function $\theta_s(n)$, evidently satisfies condition (2.1), too; it is unitary if the function $\theta_s(n)$ is real-valued.

3. Asymptotic Form of the Schrödinger Operator

The asymptotic description of the operator $T_s(\tau)$ will involve a particular one among the various unitary operators U_s , which - if it exists - can be obtained from any one of them, U_s^a , with the aid of an appropriate real valued function $\theta_s(n)$ according to formula (2.16). This particular unitary operator, denoted by W_s , is independent of τ and satisfies the condition

$$W_o = 1 . \tag{3.1}$$

Later on it will be characterized intrinsically; i.e. independently of the accidental choice of operators U_s^a . Assuming that this has been done, we can express the asymptotic behavior of the operator $T_s(\tau)$ through the formula

$$\exp\left\{ i\tau \int_o^s h_\sigma(N_o)\, d\sigma \right\} W_s^{-1} T_s(\tau) \longrightarrow 1 \quad \text{as } \tau \longrightarrow \infty; \tag{3.2}$$

the meaning of convergence involved here will be specified later on. The asymptotic description of $T_s(\tau)$ may, therefore, be given as

$$T_s(\tau) \sim W_s \exp\left\{ - i\tau\, \theta_s^o(N_o) \right\} \tag{3.3}$$

when we set

$$\theta_s^o(n) = \int_o^s h_\sigma(n)\, d\sigma \quad . \tag{3.4}$$

The superscript ^{o} is attached to the function $\theta_s(n)$ in order to distinguish this function θ from the unspecified function θ ocurring in formula (2.16) .

We shall call formula (3.3) the "adiabatic formula". Obviously, the operator $W_s \exp\left\{-i\tau\theta_s^o(N_o)\right\}$ is of the form (2.16) and thus gives a spectral transformation of the operator H_s . The adiabatic formula (3.3), therefore, implies the general adiabatic theorem.

From identity (2.10) with $b(n) = \exp\left\{-i\tau\,\theta_s^o(n)\right\}$ and $U_s = W_s$ we infer that we may write formula (3.3) also in the form

$$T_s(\tau) \sim \exp\left\{-\,i\tau\,\theta_s^o\,(N_s)\right\}\,W_s \quad , \tag{3.5}$$

which is sometimes useful, or more precisely, in the form

$$\exp\left\{i\tau\,\theta_s^o\,(N_s)\right\}\,T_s(\tau) \longrightarrow W_s \text{ as } \tau \longrightarrow \infty \ . \tag{3.6}$$

Suppose $\underline{\Phi}^{(n)}$ is an eigenstate of the label operator N_o with the point-eigenvalue $N_o = n$. Then

$$\exp\left\{-\,i\tau\,\theta_s^o(N_o)\right\}\,\underline{\Phi}^{(n)} = \exp\left\{-i\tau\,\theta_s^o(n)\right\}\,\underline{\Phi}^{(n)} \tag{3.7}$$

and formula (3.3) yields the formula

$$T_s(\tau)\underline{\Phi}^{(n)} \sim \exp\left\{ - i\tau\, e_s^o(n) \right\} W_s\underline{\Phi}^{(n)} \quad , \tag{3.8}$$

which is of the type usually given in connection with establishing the special adiabatic theorem. Note that $W_s\underline{\Phi}^{(n)}$ is an eigenfunction of N_s and hence of $H_s = h_s(N_s)$.

4. Characterization of the Transformation W_s

In the following we shall frequently use the operation, denoted by K, which transforms every unitary operator U_s into the operator

$$KU_s = i\, U_s^{-1} \nabla_s U_s \quad . \tag{4.1}$$

Here it is assumed that U_s depends on s in such a way that it possesses a continuous derivative $\nabla_s U_s$. This operator KU_s is Hermitian; i.e.

$$(KU_s)^* = KU_s \quad , \tag{4.2}$$

where the asterisk denotes the Hermitian adjoint. This fact follows from the unitary character of U_s :

$$0 = i\, \nabla_s(U_s^* U_s) = i U_s^* \nabla_s U_s + i\, \nabla_s U_s^* \cdot U_s = KU_s - (KU_s)^* .$$

At the same time we see that the derivative of the inverse $U_s^{-1} = U_s^*$ can be written in the form

$$(4.3) \qquad \nabla_s U_s^{-1} = i(KU_s)U_s^{-1} \quad .$$

For later use we also note: if the operator U_s^a is changed into

$$U_s = U_s^a \exp\left\{ i\theta_s(N_o) \right\} ,$$

see (2.16), the operator KU_s^a is changed into

$$(4.4) \qquad KU_s = KU_s^a - \nabla_s \theta_s(N_o) \quad .$$

The "intrinsic characterization" of the transformation $U_s = W_s$ can now be given in terms of the operation K : The operator $U_s = W_s$ should be such that the operator $G_s(\tau)$, defined by

$$(4.5) \qquad G_s(\tau) = \int_0^s F_\sigma(\tau)d\sigma$$

and

$$(4.6) \qquad F_s(\tau) = \exp\left\{ i\,\tau\,\theta_s^o(N_o)\right\} KW_s \exp\left\{ -\,i\,\tau\,\theta_s^o(N_o)\right\} ,$$

satisfies the condition

$$G_s(\tau) \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \tag{4.7}$$

uniformly in σ . The meaning of convergence involved here will be specified in Section 6 .

In later sections we shall consider various types of Hamiltonians and formulate "specific conditions" which insure that the transformation W_s satisfies the "intrinsic condition" (4.7) .

5. Formal Derivation of the Asymptotic Formula

In the following considerations we shall use the abbreviation

$$Y_s = \exp\left\{ - i\tau\, \theta_s^o(N_o) \right\} , \tag{5.1}$$

in which θ_s^o is given by (3.4) . We shall also omit indicating the dependence of the various operators on τ .

In order to establish relation (3.2) we introduce the operator Z_s by

$$Z_s = Y_s^{-1} W_s^{-1} T_s , \tag{5.2}$$

so that we may write the Schrödinger operator T_s in the form

$$T_s = W_s\, Y_s\, Z_s . \tag{5.3}$$

We shall then prove that the operator Z_s approaches

the identity as $\tau \rightarrow \infty$ provided the unitary operator W_s satisfies condition (4.7).

To this end we differentiate the operator Z_s with respect to s. In doing this we use relation (2.2) to write the Schrödinger equation (1.8) in the form

$$(5.4) \qquad i \nabla_s T_s = \tau h_s(N_s) T_s .$$

Using relation (2.11) for $U_s = W_s$ we may write relation (5.4) in the form

$$(5.5) \qquad i \nabla_s T_s = \tau W_s h_s(N_o) W_s^{-1} T_s .$$

Further we make use of the formula

$$(5.6) \qquad i \nabla_s Y_s^{-1} = \tau h_s(N_o) Y_s^{-1} = \tau Y_s^{-1} h_s(N_o) ,$$

which follows from (5.1) and (3.4), and finally we make use of formula (4.3) for $U_s = W_s$. Altogether we obtain the relation

$$i \nabla_s (Y_s^{-1} W_s^{-1} T_s) = Y_s^{-1} \left\{ -\tau h_s(N_o) - K W_s + \tau h_s(N_o) \right\} W_s^{-1} T_s .$$

For the operator Z_s, given by (5.2), we then obtain the equation

$$i \nabla_s Z_s = Y_s^{-1} K W_s Y_s Z_s ,$$

or

$$(5.7) \qquad i \nabla_s Z_s = F_s Z_s ,$$

when we use the operator

$$F_s = Y_s^{-1} KW_s Y_s \tag{5.8}$$

in accordance with (4.6) and (5.1) .

Integrating this relation we find the relation

$$Z_s - 1 - i \int_0^s F_\sigma (Z_\sigma - 1) d\sigma = iG_s \ , \tag{5.9}$$

in which G_s is given by (4.5) .

Relation (5.9) may be considered as a Volterra integral equation for the function $Z_s - 1$. (A similar equation was formulated by Moses [13].) Under appropriate conditions, which will be formulated in the subsequent section of the solution, this equation approaches zero whenever the right member G_s does . That this be the case is just the intrinsic condition (4.7). Hence, if this condition is satisfied, one can conclude that relation

$$(Z_s(\tau) - 1) \underline{\Phi} \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \tag{5.10}$$

holds for every state $\underline{\Phi}$. This is exactly the statement (3.2), which implies the general adiabatic theorem.

6. Rigorous Arguments

We add a few remarks about the way in which these arguments can be made rigorous. To this end we must impose various conditions on the function $h_s(n)$ and the operator W_s .

We require that the function $h_s(n)$ is continuous in s , uniformly in every bounded region of the n-space.

Instead of imposing conditions on the transformation U_s directly we impose conditions on the operator $KW_s = iW_s^{-1} \nabla W_s$ (see (4.1)).

Our primary aim is to make sure that the operator $F_s = Y_s^{-1} KW_s Y_s$, which occurs in equation (5.7), is bounded and continuous in s for $0 \leq s \leq 1$ with respect to an appropriate norm.

To this end we shall employ a norm $\|A\|$ for bounded Hermitian operators A having the property that

$$(6.1) \qquad \| g^{(1)}(N_o) A g^{(2)}(N_o) \| \leq \gamma_1 \gamma_2 \|A\|$$

whenever $g^{(1)}(n)$ and $g^{(2)}(n)$ are piecewise continuous functions of n for which

$$(6.2) \qquad |g^{(1)}(n)| \leq \gamma_1 \quad , \quad |g^{(2)}(n)| \leq \gamma_2 \ .$$

The norm

$$\|A\| = \text{l.u.b} \ \|A \Phi\| / \|\Phi\|$$

e.g. has this property. We now require first that the operator KW_s is bounded uniformly in s,[4] i.e. that there is a number $\mathcal{K}_W$ such that

$$(6.3) \qquad \| KW_s \| \leq \mathcal{K}_W \qquad \text{for} \quad 0 \leq s \leq 1 \quad .$$

With the aid of the functions

$$(6.4) \qquad g^{(1)}(n) = \exp\left\{ i\,\tau\theta_s^o(n) \right\} \quad \text{and} \quad g_s^{(2)}(n) = \exp\left\{ -\,i\tau\theta_s^o(n) \right\}$$

we may write

$$(6.5) \qquad Y_s^{-1} = g_s^{(1)}(N_o) \ , \qquad Y_s = g_s^{(2)}(N_o)$$

by (5.1), and hence, by (4.6) ,

$$(6.6) \qquad F_s = g_s^{(1)}(N_o) KW_s g_s^{(2)}(N_o) \quad .$$

Since the functions $g_s^{(1)}(n)$ and $g_s^{(2)}(n)$ satisfy condition (6.2) with $\gamma_1 = \gamma_2 = 1$, we may conclude from relation (6.1) that inequality

$$(6.7) \qquad \| F_s(\tau) \| \leq \mathcal{K}_W$$

holds for $0 \leq s \leq 1$.

---

[4] The same requirement was made by Born and Fock, who also described certain Hamiltonians for which it is satisfied.

From the assumption made about the function $h_s(n)$ it follows by (3.4) and (6.4) that the functions $g_s^{(1)}(n)$ and $g_s^{(2)}(n)$ are continuous in τ, uniformly in every bounded region of the n-space; but this continuity can not be expected to be uniform in the whole n-space. For this reason we introduce projections associated with bounded sets in n-space.

Denoting by M any bounded set in n-space we denote by P_M the projector for the operator N_o associated with this set, i.e. we set

$$(6.8) \qquad P_{\mathcal{M}} = \eta_{\mathcal{M}}(N_o)$$

where $\eta_{\mathcal{M}}(n)$ is the function for which

$$(6.9) \qquad \begin{aligned} \eta_{\mathcal{M}}(n) &= 1 \text{ if } n \text{ is in } \mathcal{M}, \\ &= 0 \text{ if } n \text{ is not in } \mathcal{M}. \end{aligned}$$

We now require secondly of the operators KW_s *that the operators* $P_{\mathcal{M}} KW_s P_{\mathcal{M}}$ *are continuous in* s *with respect to the norm introduced above and that, in addition,* $\| KW_s - P_{\mathcal{M}} KW_s P_{\mathcal{M}} \|$ *can be made arbitrarily small by proper choice of* $\mathcal{M}$ *independently of* s; i.e. to every $\varepsilon > 0$ there should be a set $\mathcal{M}(\varepsilon)$ such that

$$(6.10) \qquad \| KW_s - P_{\mathcal{M}} KW_s P_{\mathcal{M}} \| \leq \varepsilon$$

for all values of s if $\mathcal{M}$ is contained in $\mathcal{M}(\varepsilon)$.

Incidentally, it follows from these two requirements that the operator KW_s itself is continuous in s.

Since the continuity of the functions $g_s^{(1)}(n)$ and $g_s^{(2)}(n)$ of s given by (6.4) is uniform for n in $\mathcal{M}_0$, it follows that the functions $\eta_{\mathcal{M}_0}(n)g_s^{(1)}(n)$ and $\eta_{\mathcal{M}_0}(n)g^{(2)}(n)$ are uniformly continuous. Consequently, the operators $Y_s^{-1}(P_{\mathcal{M}_0})$ and $P_{\mathcal{M}_0}Y_s$ are continuous in s in the sense of the norm introduced above. At the same time we see that together with $P_{\mathcal{M}_0}KW_sP_{\mathcal{M}_0}$ also the operator $P_{\mathcal{M}_0}F_sP_{\mathcal{M}_0} = Y_s^{-1}P_{\mathcal{M}_0}KW_sP_{\mathcal{M}_0}Y_s$ is continuous in s. Finally, it follows that together with $\| KW_s - P_{\mathcal{M}_0}KW_sP_{\mathcal{M}_0} \| \leq \varepsilon$ also

(6.11) $$\| F_s - P_{\mathcal{M}_0}F_sP_{\mathcal{M}_0} \| = \| Y_s^{-1}KW_sY_s - Y_s^{-1}P_{\mathcal{M}_0}KW_sP_{\mathcal{M}_0}Y_s \| \leq \varepsilon$$

independently of s provided $\mathcal{M}_0 \supset \mathcal{M}_0(\varepsilon)$. These two properties together insure that the operator $F_s = Y_s^{-1}KW_sY_s$ is continuous in s with respect to the norm adopted for every value of τ.

We now consider the operator $Z_s = Z_s(\tau)$ which satisfies the integral equation (5.9).

We introduce the number

(6.12) $$\gamma = \gamma(\tau) = \text{l.u.b.}_s \; \| G_s \|$$

and set temporarily

(6.13) $$\zeta = \text{l.u.b.}_s \; \| Z_s - 1 \| \exp\left\{ -(1 + \kappa_W)s \right\} .$$

From relation (5.9) and (6.7) we then derive the relation

$$\| Z_s - 1 \| \leq \zeta K_W \int_0^s \exp\left\{ (1 + K_W)\sigma \right\} d\sigma + \gamma \ .$$

or

$$(6.14) \qquad \| Z_s - 1 \| \leq \zeta (1 + K_W)^{-1} K_W \exp\left\{ (1 + K_W) s \right\} + \gamma \ ,$$

whence first $\zeta \leq (1 + K_W)^{-1} K_W \zeta + \gamma$,
then

$$\zeta \leq (1 + K_W)\gamma \ .$$

Finally, by insertion into (6.14),

$$(6.15) \qquad \| Z_s - 1 \| \leq \lambda\gamma \ , \qquad 0 \leq s \leq 1 \ ,$$

with

$$(6.16) \qquad \lambda = (1 + K_W) \exp\left\{ 1 + K_W \right\} \ .$$

Condition (4.7) will now be required in the more strict form

$$(6.17) \qquad \gamma = \gamma(\tau) = \text{l.u.b.}_s \| G_s \| \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \ .$$

As a consequence of it, inequality (6.15) yields relation

$$(6.18) \qquad \text{l.u.b.}_s \| Z_s - 1 \| \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \ .$$

Thus relation (5.10), (3.2) ensue and the general adiabatic theorem is proved .

The statement of the adiabatic theorem, of course, implies the assumption that the solution T_s of the Schrödinger equation (1.9) exists. It is not obvious that this is always the case.

The fact that the differential equation $i \nabla_t T = H(t)T$ involving a non-constant, non-bounded operator H(t) has a solution if all operators H(t) have the same domain of definition was recently proved by Kato [11].

It may be indicated that also under the assumption made here the existence of the operator T_s solving equations $i \nabla_s T_s = \tau H_s T_s$, and $T_0 = 1$, could be proved for insufficiently large values of the parameter τ.

Using the estimates employed, one can show that the integral equation (5.7) possesses a solution Z_τ. The operator

$$T_s = W_s Y_s Z_s \tag{6.19}$$

is then the solution of the Schrödinger equation.

The statement of the adiabatic theorem as embodied in relation (6.18) is stronger than the statements proved by Born and Fock, and by Kato - in the case of a discrete spectrum - in as much as relation (6.18) implies that relation

$$Z_s(\tau) \underline{\Phi} \longrightarrow \underline{\Phi} \quad \text{as} \quad \tau \longrightarrow \infty \tag{6.20}$$

holds uniformly in $\underline{\Phi}$. Kato establishes this relation only for each eigen element $\underline{\Phi}^{(n)}$ of the operator H_0, while Born and Fock

prove that the matrix elements of $Z_s - 1$ approach zero ,

$$(6.21) \qquad (\underline{\Phi}^{(m)} , (Z_s - 1)\underline{\Phi}^{(n)}) \longrightarrow 0 , \quad \tau \longrightarrow \infty .$$

It would seem likely that under certain circumstances under which our strong conditions are not satisfied, relation (6.21) holds for each eigenstate $\underline{\Phi}^{(n)}$ while relation (6.8) does not hold. In such a case then the special but not the general adiabatic theorem would hold.

7. Hamiltonians with Pure Point Spectra

We proceed to formulate conditions under which the general adiabatic theorem holds in the case in which the operator N_o -- and consequently the energy operator H_o -- has a pure point spectrum.

We first assume that the eigenvalues n of the operator N_o are simple . The eigenstates for the operator N_o associated with the eigenvalues n will be denoted by $\underline{\Phi}_o^{(n)}$. The matrix elements of the operator KU_s , cf. (4.1), with respect to these eigenstates will be denoted by

$$(7.1) \qquad (n'|KU_s|n'') = (\underline{\Phi}_o^{(n')} , KU_s\underline{\Phi}_o^{(n'')})$$

We now require of the operator W_s that the diagonal terms of the matrix of KW_s vanish ,

$$(n|KW_s|n) = 0 \quad . \tag{7.2}$$

This is the "specific" condition, formulated by Fock [2], which insures that the unitary operator W_s satisfies the intrinsic condition (4.7) in case the Hamiltonian has a pure point spectrum. Additional conditions on the eigenvalues $h_s(n)$ will have to be imposed, though.

Suppose we start with an operator U_s^a for which KU_s^a does not satisfy Fock's condition. Then we may try to determine the real valued function $\theta_s^a(n)$ such that the operator

$$W_s = U_s^a \exp\left\{ i\theta_s^a(N_o) \right\} \tag{7.3}$$

does satisfy condition (7.2). Now, by (4.4), relation

$$KW_s = KU_s^a - \nabla_s \theta_s^a(N_o) \tag{7.4}$$

holds and hence

$$(n|KW_s|n) = (n|KU_s^a|n) - \nabla_s \theta_s^a(n) \quad . \tag{7.5}$$

Therefore condition (7.2) is satisfied if the function $\theta_s^a(n)$ is so determined that

$$\nabla_s \theta_s^a(n) = (n|KU_s^a|n) \quad . \tag{7.6}$$

Assuming that U_s^a is the identity for $s = 0$, the same is true of W_s if

$$\theta_o^a(n) = 0 . \tag{7.7}$$

Together with this condition, equation (7.6) determines the function $\theta_s(n)$ uniquely. Note that $(n|KU_s^a|n)$ is real since KU_a^a is Hermitian as was shown above, see (4.2) .

Incidentally, as Fock has observed [2], condition (7.2) can be written in the concise form

$$\left(\underline{\Phi}_s^{(n)} , \nabla_s \underline{\Phi}_s^{(n)} \right) = 0 \tag{7.8}$$

in terms of the eigenstates $\underline{\Phi}_s^{(n)} = U_s \underline{\Phi}_o^{(n)}$.

Of the eigenvalues $h_s(n)$ of the energy operator H_s we require that they are positive and different from each other. Accordingly, two different branches $h_s(n')$ and $h_s(n'')$ of the set of eigenvalues are not permitted to cross or even to meet.

This condition is stronger than necessary. Born and Fock assume only that each of the functions $h_s(n') - h_s(n'')$ vanishes at most at a finite number of values $s = s_o$ and satisfies the inequality $|h_s(n') - h_s(n'')| \geq c|s - s_o|^r$ there. (In fact they weaken even the continuity requirement of KW_s). They then show that the matrix elements of $Z_s(\tau) - 1$ are of the order of magnitude $\tau^{-1/r+1}$. Kato does not specify the order of magnitude of $h_s(n') - h_s(n'')$ and accordingly deduces only the relation $Z_s(\tau)\, \underline{\Phi}^{(n)} \longrightarrow \underline{\Phi}^{(n)}$. If one wanted to prove the uniform statement $\| Z_s(\tau) - 1 \| \longrightarrow 0$ as $\tau \longrightarrow \infty$, one would have to slightly strengthen these weakened conditions. We shall

not investigate this problem in general, but in Part II we shall treat in detail this problem for $r = 1$, assuming the Hilbert space of states to be two-dimensional.

We proceed to show that the intrinsic condition (4.7) $G_s = G_s(\tau) \longrightarrow 0$ as $\longrightarrow \infty$, is satisfied in the form (6.17) if the specific condition (7.2) is satisfied.

To this end we consider the N_o-matrix element of the operator G_s,

$$(7.9) \quad (n'|G_s|n'') = \int_o^s (n'|KW_{s'}|n'')\exp\left\{i\tau^{-1}\int_o^{s'}[h_s(n')-h_\sigma(n'')]d\sigma\right\}d\sigma'$$

If $n' = n''$ this matrix element vanishes,

$$(7.10) \qquad (n|G_s|n) = 0 ,$$

by virtue of the basic assumption (7.2). If $n' \neq n''$, on the other hand we may introduce the variable

$$\alpha = \int_o^s [h_\sigma(n') - h_\sigma(n'')]d\sigma$$

instead of s and consider $s = s(\alpha)$ as a function of α. For, $h_s(n') \neq h_s(n'')$ for $n' \neq n''$ and $0 \leq s \leq 1$ was assumed.

In terms of the independent variable α' the matrix element (7.9) can be written in the form

$$(7.11) \quad (n'|G_s|n'') = \int_o^\alpha (n'|KW_{s'}|n'')\exp\left\{i\tau^{-1}\alpha'\right\}[h_{s'}(n')-h_{s'}(n'')]^{-1}d\alpha$$

From the assumed continuous dependence of the operator KW_s on s , it follows that the matrix element $(n'|KW_s|n'')$ is continuous in s . Therefore, one may infer from (7.11) that the matrix element $(n'|G_s(\tau)|n'')$ approaches zero as τ approaches ∞ ,

$$(7.12) \qquad (n'|G_s(\tau)|n'') \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \ .$$

This fact now implies that the operator $P_{\mathcal{M}}G_sP_{\mathcal{M}}$ approaches zero. For, the operator $P_{\mathcal{M}}$, defined by (6.8), projects into a finite dimensional space and, therefore, the operator $P_{\mathcal{M}}G_sP_{\mathcal{M}}$ involves only a finite number of matrix elements (7.11); namely those for which n' and m' belong to the set $\mathcal{M}$. This statement may also be put in the form

$$(7.13) \qquad \| P_{\mathcal{M}} G_sP_{\mathcal{M}} \| \longrightarrow 0 , \quad \text{as} \quad \tau \longrightarrow \infty$$

since for a finite matrix it does not matter which norm is taken.

On the other hand, from the assumed property (6.1) of the norm and from (6.10) one can derive the inequality

$$(7.14) \qquad \| G_s - P_{\mathcal{M}} G_sP_{\mathcal{M}} \| \leq \text{l.u.b.}_s \| KW_s - P_{\mathcal{M}} KW_sP_{\mathcal{M}} \| \leq \varepsilon$$

for $\mathcal{M} \supset \mathcal{M}(\varepsilon)$. Together with (7.13) this fact leads to the relation

$$(7.15) \qquad \| G_s(\tau) \| \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \ .$$

Thus it is established that the intrinsic condition (4.7) is satisfied and the validity of the adiabatic theorem follows.

It should be mentioned that for his problem Kato [7] characterizes the operator W_s not by condition (7.2) but in a different way. He introduces the projectors $E_s^{(n)}$ associated with the operator H_s and the eigenvalue $h_s^{(n)}$ and then determines the operator W_s as a solution of the differential equation

$$(7.16)\qquad \nabla_s W_s = \frac{1}{2} \sum_n \left[\dot{E}_s^{(n)} E_s^{(n)} - E_s^{(n)} \dot{E}_s^{(n)} \right] W_s$$

with $\nabla_s E_s^{(n)} = \dot{E}_s^{(n)}$ assumed to exist continuously. It is easily verified that any operator W_s which satisfies this differential equation and the condition $W_o = 1$ is unitary and satisfies the relation

$$(7.17)\qquad E_s^{(n)} W_s = W_s E_o^{(n)} \quad .$$

By virtue of relation (7.16) the operator KW_s becomes

$$KW_s = \frac{1}{2} W_s^{-1} \sum_n \left[\dot{E}^{(n)} E^{(n)} - E^{(n)} \dot{E}^{(n)} \right] W_s \quad ;$$

further

$$(n'|KW_s|n') = (E_o^{(n')}, KW_s E_o^{(n')})$$

$$= \frac{1}{2} W_s^{-1} E_s^{(n')} \sum_n \left[\dot{E}_s^{(n)} E_s^{(n)} - E_s^{(n)} \dot{E}_s^{(n)} \right] E_s^{(n')} W_s = 0$$

since $E_s^{(n)}E_s^{(n')} = 0$ if $n' \neq n$, $= E_s^{(n)}$ if $n' = n$. Thus it is seen that Kato's operator satisfies condition (7.2).

8. Asymptotic Expansion

We proceed to indicate how one can obtain the asymptotic expansion of the Schrödinger operator T_s, of which the general adiabatic theorem gives the term of lowest order.

In Section 5 we wrote the operator T_s in the form

$$T_s = W_s Y_s Z_s \tag{5.3}$$

and proved that Z_s approaches the identity when $\tau \longrightarrow \infty$. For the purpose of an asymptotic expansion of $T_s = T_s(\tau)$ it is more appropriate to write this operator in a different form. To this end one should introduce solutions ψ_s of the Schrödinger equation

$$i \nabla_s \psi_s = \tau H_s \psi_s \tag{8.1}$$

which do not necessarily reduce to the identity for $s = 0$. The operator $\psi_s \psi_0^{-1}$ then does reduce to the identity for $s = 0$; since this operator is also a solution of the Schrödinger equation, it is the operator T_s,

$$T_s = \psi_s \psi_0^{-1} . \tag{8.2}$$

One should now write the operator ψ_s in the form

$$(8.3) \qquad \psi_s = W_s J_s Y_s$$

and determine an asymptotic expansion of the operator J_s.

This is motivated by the analogy with the results of the theory of asymptotic expansion of solutions of ordinary differential equations -- cf. e.g. [13]. In fact, according to this analogy one should expect that the operator J_s could be so determined that it possesses an asymptotic power series expansion of the form

$$(8.4) \qquad J_s(\tau) \sim \sum_{K=0}^{\infty} \tau^{-K} J_s^{(K)} \quad .$$

We shall not actually prove the possibility of such an expansion rigorously, but shall be satisfied with describing the procedure for determining the coefficients $J_s^{(K)}$ formally.

As seen from relations (5.4), (5.5), (5.6), the matrix J_s satisfies the equation

$$(8.5) \qquad i \nabla_s J_s = \tau \left[h_s(N_o) J_s - J_s h_s(N_o) \right] + K_s J_s \quad ,$$

in which

$$(8.6) \qquad K_s = K W_s \ ,$$

cf. (4.1), while $h_s(N_o)$ was defined in Section 2. After insertion of the expansion (8.4) into equation (8.5) it is seen that the operator $J_s^{(K)}$ should satisfy the conditions

$$(8.7)_o \qquad \left[h_s(N_o)J_s^{(o)} - J_s^{(o)}\, h_s(N_o)\right] = 0 \;,$$

$$(8.7) \qquad \left[h_s(N_o)J_s^{(K+1)} - J_s^{(K+1)}h_s(N_o)\right] = i\nabla_s J_s^{(K)} - K_s J_s^{(K)}, \; K \geq 0 \;.$$

We want to show that it is possible to determine the operator $J_s^{(K+1)}$ successively from equation (8.5) at least formally.

We express equation (8.5) as the equality of the matrix elements - with respect to the label operator N_o - of both sides of it:

$$(8.8) \; \left[h_s(n') - h_s(n'')\right] \; (n'|J_s^{(K+1)}|n'') = (n'|i\nabla_s J_s^{(K)} - K_s J_s^{(K)}|n'')$$

Since the left member vanishes for $n' = n''$, the diagonal term of the right member vanishes, too:

$$(8.9) \qquad (n|i\nabla_s J_s^{(K)} - K_s J_s^{(K)}|n) = 0 \;.$$

Evidently, one must satisfy condition (8.9) before one can determine $J_s^{(K+1)}$ from equation (8.7) .

Suppose the operator $J_s^{(K)}$ has been so determined that relation (8.9) holds. Then we introduce an operator $\overset{o}{J}{}_s^{(K+1)}$ which has the matrix elements

(8.10)

$$(n'|\overset{o}{J}{}_s^{(K+1)}|n'') = \left[h_s(n')-h_s(n'')\right]^{-1}(n'|i\nabla_s J_s^{(K)} - K_s J_s^{(K)}|n'')$$

$$\text{for} \;\; n' \neq n'' \;,$$

$$(n|\overset{o}{J}{}_s^{(K+1)}|n) = 0 \quad . \tag{8.11}$$

Note that $h_s(n') \neq h_s(n'')$ for $n' \neq n''$, as assumed in Section 2 . It is then clear that the operator $\overset{o}{J}{}_s^{(K+1)}$, in place of $J_s^{(K+1)}$, satisfies equation (8.8) .

The diagonal terms of $J_s^{(K+1)}$ are evidently not determined by condition (8.8). In fact, $J_s^{(K+1)}$ is uniquely determined by equation (8.8) only except for the addition of an arbitrary operator which commutes with $h_s(N_o)$, and hence is a function of N_o . Thus we may write

$$J_s^{(K+1)} = \overset{o}{J}{}_s^{(K+1)} + \alpha_s^{(K+1)}(N_o) \tag{8.12}$$

with an appropriate function $\alpha_s^{(K+1)}(n)$.

We shall show that this function can be so determined that condition (8.9), for $K + 1$ instead of K , is satisfied. After inserting (8.9) into this condition, we observe that two of the resulting four terms drop out. First we note that relation (8.12) implies

$$(n|\nabla_s \overset{o}{J}{}_s^{(K+1)}|n) = \nabla_s (n|J_s^{(K+1)}|n) = 0 \; .$$

Secondly we note that relation (7.2), which by (8.6) can be written as

$$(n|K_s|n) = 0 \quad , \tag{8.13}$$

implies the relation

$$(n|K_s \alpha_s^{(K+1)}(N_o)|n) = (n|K_s|n)\alpha_s^{(K+1)}(n) = 0 .$$

Hence, insertion of (8.11) into (8.9) yields equation

$$i\nabla_s \alpha_s^{(K+1)}(n) = (n|K_s \overset{o}{J}{}_s^{(K+1)}|n) , \tag{8.14}$$

from which the function $\alpha_s^{(K+1)}(n)$ may be determined.

We begin our process with the matrix

$$J^{(o)} = 1 , \tag{8.15}$$

which evidently satisfies equation $(8.7)_o$. It also satisfies condition (8.9) for $K = 0$ by virtue of (8.13) . It is then clear that our process of determining the operators $J_s^{(K+1)}$ successively can be carried out formally.

Let us, in particular, consider the second approximation,

$$J_s \sim 1 + \tau^{-1} J_s^{(1)} . \tag{8.16}$$

To second order we may just as well set

$$(8.17)_1 \qquad J_s \sim \exp\left\{ \tau^{-1} J_s^{(1)} \right\} \qquad \text{or}$$

$$(8.17)_2 \qquad J_s \sim \exp\left\{ \tau^{-1} \overset{o}{J}{}^{(1)} \right\} \exp\left\{ \tau^{-1} \alpha_s(N_o) \right\} .$$

By (8.3) we hence may write

$$(8.18) \qquad \psi_s \sim W_s \exp\left\{\tau^{-1}\overset{o}{J}{}_s^{(1)}\right\} \exp\left\{\tau^{-1}\alpha_s(N_o) - i\,\tau\, e_s^{(o)}(N_o)\right\} \quad .$$

It would not be difficult to show that the operators $i\overset{o}{J}{}_s^{(1)}$, $i\alpha_s(N_o)$ and hence $iJ_s^{(1)}$ are Hermitian if, in integrating equation (8.12) for K = 0, the initial value of $\alpha_s^{(1)}(n)$ is chosen $\alpha_o^{(1)}(n) = 0$. Hence all exponential function occurring in (8.17) (8.18) are unitary operators.

For $s = 0$ we have $W_o = 1$ by (3.1) , $e_o^{(o)}(n) = 0$ by (3.4) , and $\alpha_o^{(1)}(n) = 0$ as assumed above; hence we have

$$(8.19) \qquad \psi_o \sim \exp\left\{\tau^{-1}\overset{o}{J}{}_o^{(1)}\right\}$$

and hence by (8.3)

$$(8.20) \quad T_s \sim W_s \exp\left\{\tau^{-1}\overset{o}{J}{}_s^{(1)}\right\} \exp\left\{\tau^{-1}\alpha_s(N_o) - i\,\tau\,\theta_s^{(o)}(N_o)\right\} \exp\left\{-\,\tau^{-1}\overset{o}{J}{}_o^{(1}\right.$$

Each of these exponential functions is evidently Hermitian .

The considerations in this section are purely formal. Nevertheless, we shall indicate how one could prove the validity of the asymptotic expansion up to the order K , once the terms $J^{(K)}$ up to this order have been determined.

We introduce an operator $Z^{(K)}$ by setting

$$(8.21) \qquad \psi_s = W_s \left\{ \sum_{\kappa=o}^{K} \tau^{-\kappa} J_s^{(\kappa)} Y_s + \tau^{-K} Y_s Z_s^{(K)} \right\} \quad .$$

Insertion into equation (8.1) and use of equation (8.7) yields equation

(8.22) $$i \nabla_s Z_s^{(K)} - F_s Z_s^{(K)} = F_s^{(K)}$$

for $Z_s^{(K)}$, in which

(8.23) $$F_s^{(K)} = Y_s^{-1} \left[K_s J_s^{(K)} - i \tilde{\nabla}_s J_s^{(K)} \right] Y_s$$

and, cf. (4.6), (8.15) ,

(8.24) $$F_s = F_s^{(1)} \quad .$$

With

(8.25) $$G_s^{(K)} = \int_0^s F_\sigma^{(K)} \, d\sigma \quad ,$$

cf. (4.5), we obtain the integral equation

(8.26) $$Z_s^{(K)} - \int_0^s F_\sigma Z_\sigma^{(K)} \, d\sigma = i G_s^{(K)}$$

for $Z_s^{(K)}$, which is of the same type as equation (5.9) for the operator $Z_s - 1$. Under appropriate conditions, similar to those formulated in Section 6, one can prove the existence of an operator $Z_s^{(K)}$ which satisfies condition (8.26) and which approaches zero with τ^{-1} ,

$$Z_s^{(K)}(\tau) \, \underline{\Phi} \longrightarrow 0 \quad \text{as} \quad \tau \longrightarrow \infty \quad .$$

The operator ψ_s defined by (8.21) then satisfies the Schrödinger equation (8.1) and possesses the asymptotic expansion

$$\psi_s \sim W_s \sum_{\kappa=0}^{K} \tau^{-\kappa} J_s^{(\kappa)} Y_s \tag{8.27}$$

up to the order K .

9. Hamiltonian Operators With Continuous Spectra

We proceed to discuss the adiabatic theorem in cases where the energy operators have continuous spectra. We make several simplifying assumptions. We first assume that the spectrum of H_o is purely continuous, extending over a half-infinite interval $\mu \leq h \leq \infty$; here μ is a positive number. Moreover, we assume that for all values of s the spectra of the operators H_s are the same, including multiplicities. Accordingly, we may take as label operator N_s the energy H_s itself together with appropriate "angular" variables A_s ,

$$N_s = \left\{ H_s , A_s \right\} . \tag{9.1}$$

The eigenvalues of H_s and A_s will be denoted by h and a ; the eigenvalue of N_s is then

$$n = \left\{ h, a \right\} . \tag{9.2}$$

The function $h_s(n)$, used to express the operator H_s as $H_s = h_s(N_s)$ in terms of N_s , see (2.2), now simply becomes

$$(9.3) \qquad h_s(h,\alpha) = h ;$$

it is evidently independent of s . Similar variables h and α were used by Snyder [9] .

Relation (2.1) now takes the form

$$(9.4) \qquad H_s = U_s H_o U_s^{-1} ,$$

$$(9.5) \qquad A_s = U_s A_o U_s^{-1} .$$

It is sufficient to make sure that relation (9.4) can be satisfied by an appropriate unitary operator U_s ; relation (9.5) may then simply serve to define the operator A_s in terms of A_o .

Precise conditions on the disturbance operator

$$(9.6) \qquad V_s = H_o - H_s$$

under which a unitary operator U_s exists such that relation (9.4) holds were formulated in earlier papers [3,5] . A class (R) of operators Q was introduced by the condition that the functional operator Q can be an integral operator Q of the class (R) the operator $\Gamma_- Q$ whose N_o - representer is a singular integral operator with a symbolic kernel which can be written in the form

$$(9.9)_- \qquad (h,\alpha| \Gamma_- Q|h',\alpha') = 2\pi i\delta_-(h-h')(h,\alpha|Q|h',\alpha') ,$$

in which the abbreviation

$$(9.10)_{\pm} \qquad \delta_{\pm}(z) = \frac{1}{2}\,\delta(z) \pm \frac{1}{2i\pi z}$$

has been used. The operator Γ_+ is obtained from Γ_- by substituting $-i$ for i ,

$$(9.9)_{+} \qquad (h,\alpha|\Gamma_+ Q|h',\alpha') = 2\pi i\delta_+(h-h')(h,\alpha|Q|h',\alpha) \quad .$$

Among the various equivalent unitary operators U_s there is one which is of the form

$$(9.11) \qquad W_s = 1 + \Gamma_- R_s$$

in which R_s is an integral operator of class (R) . This fact was also proved earlier [3,5] . We have used the notation W_s for this special operator U_s because, as we shall show, *the operator W_s is the one that enters the asymptotic description (3.3) of the Schrödinger operator* $T_s(\tau)$.

Before we can describe the special form of formula (3.3) in the present case, we must determine the special form of the expression $\theta^0_s(n)$ defined by (3.4). Since the function $h_s(h,\alpha) = h$ is independent of s, cf. (9.3), the angle θ^0_s defined by (3.4) is found as

$$(9.12) \qquad \theta^0_s(h,\alpha) = sh \quad .$$

Consequently, *the adiabatic formula* (3.3) takes the form

$$(9.13) \qquad T_s(\tau) \sim (1 + \Gamma_- R_s)\exp\left\{-i\tau sH_0\right\} \quad .$$

In order to establish this formula we must investigate the properties of the operator KW_s . To this end we first note that the inverse of W_s is given by its adjoint

$$W_s^{-1} = 1 - \Gamma_- R_s^* \quad ; \tag{9.14}$$

here R_s^* is the Hermitian adjoint of R_s . Secondly we state: under appropriate conditions concerning the dependence of the operator R_s on the parameter s, the operator R_s has a continuous derivative $\nabla_s R_s$ of class (R) such that the derivative

$$\nabla_s W_s = \Gamma_- \nabla_s R_s \tag{9.15}$$

has the properties stipulated earlier.

In view of the definition (4.1) the operator KW_s appears first in the form

$$KW_s = i(1 - \Gamma_- R_s^*)\Gamma_- \nabla_s R_s \quad . \tag{9.16}$$

We may, however, make use of the fact that the operators $F_1 \Gamma_- F_2, \Gamma F_1 \cdot F_2$ are of class (R) and that the identity

$$\Gamma_- F_1 \Gamma_- F_2 = \Gamma_- \left[F_1 \Gamma_- F_2 + \Gamma_- F_1 \cdot F_2 \right] \quad , \tag{9.17}$$

holds,[5] [3,4]. Accordingly, we may write the operator KW_s in the form

---

[5] See remark II in the appendix.

$$(9.18) \qquad KW_s = \Gamma_- P_s \quad ,$$

in which the operator

$$(9.19) \qquad P_s = i\nabla_s R_s - iR_s^* \Gamma_- \nabla_s R_s - i(\Gamma_- R_s^*)\nabla_s R_s$$

is again of class (R). It is the form (9.18) of the operator KW_s which is decisive for the following argument.

The main step in establishing formula (9.13) consists in showing that with the choice (9.11) of the unitary operator W_s, relation (4.7) holds, $G_s(\tau) \longrightarrow 0$ as $\tau \longrightarrow \infty$. To this end it is sufficient to prove that relation $F_s(\tau) \longrightarrow 0$ as $\tau \longrightarrow \infty$ holds for $s > 0$. The operator F_s, defined by (4.6), assumes a particularly simple form in the present problem, namely

$$(9.20) \qquad F_s(\tau) = \exp\left\{ i\tau s H_o \right\} KW_s \exp\left\{ -i\tau s H_o \right\} \quad ,$$

as is seen from (9.12).

Now, one of the main properties of the operation Γ_- is expressed in the relation

$$(9.21) \qquad \exp\left\{ itH_o \right\} \Gamma_- Q \exp\left\{ -itH_o \right\} \longrightarrow 0 \qquad \text{as } t \longrightarrow \infty \; ,$$

see [5, 4].[6]

---

[6] It is equivalent with the statement

$$\int \delta_-(h-h')(h,a|Q|h',a')\exp\left\{ it(h-h') \right\} \psi(a',h')dm(a')dh' \longrightarrow \infty$$
$$\text{as } t \longrightarrow \infty \; .$$

Since by (9.18) the operator KW_s is of the form $\underline{\Gamma} P_s$, relation

$$(9.22) \qquad F_s(\tau) \longrightarrow 0 \quad \text{as } \tau \longrightarrow \infty , \quad \text{for } s > 0 ,$$

ensues and hence (5.7) holds. The asymptotic formula (3.3) in the form (9.13) is thus essentially established.

By using the notions employed earlier [4, 6], it would not be difficult to make the foregoing arguments rigorous and to establish relation (5.7) in the strict sense (7.15). We refrain from doing so.

10. Asymptotic Behavior of the Schrödinger Operator

The adiabatic formula (9.13) stands for the relation

$$(10.1) \qquad \exp\left\{ i\tau\, sH_o \right\} (1 + \underline{\Gamma} R_s)^{-1} T_s(\tau) \longrightarrow 1 \quad \text{as} \quad \tau \longrightarrow \infty .$$

Since identity (9.4) implies identity

$$(10.2) \qquad (1 + \underline{\Gamma} R_s) \exp\left\{ i\tau\, sH_o \right\} = \exp\left\{ i\tau\, sH_1 \right\} (1 + \underline{\Gamma} R_s)$$

relation (10.1) is equivalent to the relation

$$(10.3) \qquad \exp\left\{ i\tau\, sH_1 \right\} T_s(\tau) \longrightarrow (1 + \underline{\Gamma} R_s) \quad \text{as} \quad \tau \longrightarrow \infty ,$$

cf. (3.2) and (3.6), or simply to the relation

$$(10.4) \qquad T_s(\tau) \sim \exp\left\{ -i \quad sH_1 \right\} (1 + \underline{\Gamma} R_s) \quad .$$

For $s = 1$, in particular, this formula becomes

$$T_1(\tau) \sim \exp\left\{-i\tau H_1\right\}(1 + \Gamma_- R_1) \quad . \tag{10.5}$$

This formula is of particular significance in the case where the operator H_o is considered as a "disturbed" and the operator H_1 as the "undisturbed" Hamiltonian. For, in this case formula (10.4) answers the question how one can express the Schrödingerstate $T_1(\tau)\,\Phi^{(o)}$ at the time t_1 approximately in terms of the undisturbed operator H_1 .

In deriving formula (10.5) it was assumed that the disturbance $H_o - H_1$ is switched off during the time interval from $t = t_o$ to $t = t_1 = t_o + \tau$. The assumption that the disturbance is switched off one way or the other would naturally seem to be essential for the validity of formula (10.4) . It is remarkable that this is not so.

Suppose the disturbed Hamiltonian H_o is kept constant. Then the Schrödinger operator is simply $\exp\left\{-i(t - t_o)H_o\right\}$.

Now from relation (10.2) for $s = 1$ and (9.14) we deduce the relation

$$\exp\left\{i\tau H_1\right\} = (1 + \Gamma_- R_1)\exp\left\{i\tau H_o\right\}(1 - \Gamma_- R_1^*) \quad ,$$

whence by (9.21) with $Q = R_1^*$

$$\exp\left\{i\tau H_1\right\}\exp\left\{-i\tau H_o\right\} \longrightarrow 1 + \Gamma_- R_1 \quad \text{as} \quad \tau \longrightarrow \infty \tag{10.6}$$

or

$$(10.7) \qquad \exp\left\{-i\,\tau\,H_o\right\} \sim \exp\left\{-i\,\tau\,H_1\right\}\,(1 + \Gamma_- R_1) \quad .$$

The fact, expressed through formula (10.6), that relation (10.4) holds even if the disturbance $H_o - H_1$ is not switched off was called by Snyder [9] the "irrelevancy of the adiabatic hypothesis".

The questions just discussed arise in problems of scattering. As mentioned above, the operator H_o , the actual Hamiltonian at the time $t = 0$, plays the role of the disturbed operator, while H_1 , the Hamiltonian to be acting after infinite time, is the undisturbed energy operator. Instead of speaking of producing the undisturbed operator, one prefers to speak of switching the disturbance $H_o - H_1$ off.

Suppose one wants to investigate the switching-on of the disturbance by letting the initial time approach $-\infty$ while keeping the end time fixed. Then one may use the same formulas that we have given, letting t_o be the end time and t_1 the initial time. The Schrödinger operator which describes the transition from the initial time t_1 to the end time t_o is then the inverse $T_1^{-1}(\tau)$ of the operator $T_1(\tau)$. The only place in which the sign of $\tau = t_1 - t_o$ matters is the formula (9.21). In its place, formula

$$(10.8) \qquad \exp\left\{itH_o\right\}\,\Gamma_+ Q\,\exp\left\{-itH_o\right\} \longrightarrow 0 \quad \text{as} \quad t \longrightarrow -\infty ,$$

should be used, in which instead of Γ_- the operation Γ_+ occurs, cf. (9.9). Accordingly, all formulas given remain valid for $\tau \longrightarrow -\infty$ if everywhere Γ_- is replaced by Γ_+, and at the same time R is replaced by an appropriate other operator R in the class (R) . Thus the adiabatic formula

$$(10.9) \quad T_s(\tau) \sim (1 + \Gamma_+ R_s) \exp\left\{-i\tau sH_0\right\} = \exp\left\{-i\tau sH_1\right\}(1 + \Gamma_+ R_s)$$

is obtained from (9.13) and (10.4). Its inverse for $s = 1$

$$(10.10) \quad T_1^{-1}(\tau) \sim \exp\left\{i\tau sH_0\right\}(1 - \Gamma_+ R^*) = (1 - \Gamma_+ R^*)\exp\left\{i\tau sH_1\right\}$$

describes asymptotically the Schrödinger operator $T_1^{-1}(\tau)$ for the process in which the disturbed energy operator H_0 is produced infinitely slowly at the time t_0 from the undisturbed energy operator H_1 acting at the initial time $t_1 \sim -\infty$. From formula

$$(10.11) \qquad \exp\left\{i\tau H_1\right\} \exp\left\{-i\tau H_0\right\} \longrightarrow 1 + \Gamma_+ R_1 \quad \text{as} \quad \tau \longrightarrow -\infty ,$$

the counterpart of formula (10.6), one again infers the irrelevancy of the adiabatic hypothesis for the switching-on process.

11. A Problem From the Quantum Theory of Fields

We proceed to discuss the adiabatic formulas in the case of a simple problem which occurs in the quantum theory of fields. Except for one point eigenvalue, the spectrum of the energy operator may be continuous in this problem. Nevertheless, the unitary operator W will be determined according to a rule which closely corresponds to the rule (7.2) for point spectra and not to the rule (9.11) for continuous spectra. In fact, the spectrum of the label operator behaves essentially like a point spectrum, as will be seen, and this feature dominates. The correctness of the result so obtained can be verified since the Schrödinger equation can be solved explicitly in this case.

The problem concerns the behavior of a boson field under the influence of a charge distribution which is a given function of time t and position x, [10] .

The problem involves functions of a certain "single particle observable", denoted by p , which should be so chosen that the "single particle energy" h is a function of it,

$$h = h(P) \quad . \tag{11.1}$$

In general, the momentum may serve as variable p and then $h(p) = (\mu^2 + |p|^2)^{1/2}$ with an appropriate constant $\mu > 0$. This interpretation of p , however, is not essential in the following.

The "field" can now be characterized by a pair of

"creation and annihilation operators" $A^{+}(p,t)$ and $A^{-}(p,t)$, which depend on p and the time t. The operators to which $A^{\pm}(p,t)$ reduce for the initial time $t = t_o = 0$, denoted by $A^{\pm}(p)$, are assumed to be given

$$A^{\pm}(p,0) = A^{\pm}(p) \quad . \tag{11.2}$$

The operators $A^{\pm}(p,t)$ are to be solutions of the differential equation

$$(\pm i \nabla_t + h)A^{\pm}(p,t) = hq^{\pm}(p,t) \tag{11.3}$$

with $h = h(p)$. Here $q^{\pm}(p,t)$ is a pair of complex conjugate functions connected with the given charge distribution. The initial operators $A^{\pm}(p)$ are to satisfy certain commutation rules to be formulated presently.

Let $b_1^{\pm}(p)$, $b_2^{\pm}(p)$ be two pairs of complex conjugate functions. Then we introduce the abbreviations

$$b_1^{+}b_2^{-} = \int b_1^{+}(p)b_2^{-}(p)dp \quad ; \tag{11.4}$$

here the integration is to be extended over the whole p-space. We also introduce the operators

$$A^{+}b^{-} = \int A^{+}(p)b^{-}(p)dp \quad , \quad b^{+}A^{-} = \int b^{+}(p)A^{-}(p)dp \quad ; \tag{11.5}$$

they should obey the commutation rules

(11.6) $$[b_1^+A^- , A^+b_2^-] = b_1^+b_2^- ,$$

(11.7) $$[b_1^+A^- , b_2^+A^-] = [A^+b_1^- , A^+b_2^-] = 0 .$$

In the following we also need the operator

(11.8) $$A^+hA^- = \int A^+(p)h(p)A^-(p)dp ,$$

which obeys the commutation rule

(11.9) $$[b^+A^-, A^+hA^-] = b^+hA^- ,$$

$$[A^+hA^- , A^+b^-] = A^+hb^- .$$

The solutions of equations (11.3) can , of course, be given explicitly.

(11.10) $$A^\pm(p,t) = \exp\left\{ \pm ith \right\} [A^\pm(p) - g^\pm(p,t)]$$

with

(11.11) $$g-(p,t) = \int_0^t \pm ih \exp\left\{ \mp it'h \right\} q^\pm(p,t')dt' .$$

One of the main tasks in the theory is to express the operators $A^\pm(p,t)$ in terms of $A^\pm(p)$ with the aid of a canonical transformation $T(t)$,

(11.12) $$A^\pm(p,t) = T^{-1}(t)A^\pm(p)T(t)$$

Such a transformation can be found as the solution of the Schrödinger equation

$$(11.13) \qquad i\nabla_t T(t) = H(t)T(t) \quad , \qquad T(0) = 1 \quad ,$$

in which the Hamiltonian $H(t)$ is given by

$$(11.14) \qquad H(t) = (A^{+} - q^{+}(t)h(A^{-} - q^{-}(t)$$

$$= A^{+}hA^{-} - A^{+}hq^{-}(t) - q^{+}(t)hA^{-} + q^{+}(t)hq^{-}(t) \quad .$$

Note that this Hamiltonian $H(t)$ is expressed in terms of the operators $A^{\pm}(p)$ at the initial time $t = 0$, see (11.2), in accordance with the general quantum theoretical formalism. Cf. footnote 2 .

Suppose we define the operators $A^{\pm}(p,t)$ by (11.12) taking for $T(t)$ the solution of (11.13). Then we find that the function $A^{\pm}(p,t)$ satisfies the equation

$$(11.15) \qquad i\nabla_t A^{\pm}(p,t) = [A^{\pm}(p), H(t)] \quad .$$

We insert the definition (11.14) of $H(t)$ and employ the commutation rules (11.6), (11.7), (11.9) . Then equation (11.15) reduces to equation (11.3). Thus it is seen that the solution of (11.13) yields that of (11.3).

We now consider a set of functions $q^{\pm}(t) = q^{\pm}(p,t)$, given by

$$(11.16) \qquad q^{\pm}(t) = q^{\pm}_{t} \qquad \text{for} \quad 0 \leq t \leq \tau$$

$$= 0 \qquad \text{for} \quad \tau \leq t \quad ,$$

in which $q_s^{\pm}$ is a given function of s for $0 \leq s \leq 1$ with

$$q_1^{\pm} = 0 \quad . \tag{11.17}$$

In other words, we switch off the external field arbitrarily slowly. We then try to find an approximate description of the Schrödinger operator

$$T(t) = T_s(\tau) \quad .$$

To this end, according to the general theory developed, we should first describe label operators N_s . We recall that the symbol N_s was not necessarily restricted to mean a single operator; it just as well could represent a system of a finite number of commuting operators. It is not possible to set up such a finite system in the present problem. It is, however, possible to set up infinite such systems. Therefore, the theory developed is not applicable in a strict sense and the following considerations can have only a heuristic significance. We find it convenient to let N_s stand for an infinite set of operators which have only a symbolic meaning; this should not be objectionable since our argument is only heuristic anyway. (As mentioned above the validity of the results will be established from an explicit expression for the Schrödinger operator.)

To each value of p one of these symbolic operators is assigned, namely the operator

$$N_s(p) = \left(A^+(p) - q_s^+(p)\right)\left(A^-(p) - q_s^-(p)\right)dp \quad . \tag{11.18}$$

Observe the absence of an integral sign. Each of these operators $N_s(p)$ has a pure point spectrum consisting of the eigenvalues $\nu(p) = 0,1,2,\ldots$. Actually, the numbers $\nu(p)$ are nothing but the occupation numbers, cf. [10] . The fact that each of these operators has a point spectrum indicates that for the determination of the operator W_s the rule for point spectra should be adopted.

The operator H_s can be expressed as a function of the operator $N_s(p)$ in the form

$$H_s = \sum_p h(p)\, N_s(p) \quad . \tag{11.19}$$

The function $h_s(n)$ should therefore be replaced by the functional

$$h_s\{\nu\} = \sum_p h(p)\, \nu(p) \tag{11.20}$$

of the occupation numbers $\nu(p)$. This functional h_s is evidently independent of s .

The next step consists in determining the unitary operator U_s such that

$$N_s(p) = U_s\, N_o(p)\, U_s^{-1} \quad , \tag{11.21}$$

for each p , cf. (2.1). To this end it is sufficient to determine the unitary operator U_s such that

$$A^{\pm}(p) - q_s^{\pm}(p) = U_s\left(A^{\pm}(p) - q_o^{\pm}(p)\right)U_s^{-1} \tag{11.22}$$

or, more properly,

$$(11.23) \qquad b^{+}(A^{-} - q_s^{-}) = U_s b^{+}(A^{-} - q_o^{-})U_s^{-1} \ ,$$

$$(A^{+} - q_s^{+})b^{-} = U_s(A^{+} - q_s^{+})b^{-}U_s^{-1} \ .$$

Such a transformation U_s can be given in the form

$$(11.24) \qquad U_s = \exp\left\{A^{+}(q_s^{-} - q_o^{-}) - (q_s^{+} - q_o^{+})A^{-}\right\} \ ,$$

see [10] .

We proceed to determine the transformation

$$(11.25) \qquad W_s = U_s \exp\left\{i\theta_s\right\}$$

which will enter the asymptotic description of $T(t)$. In order to determine θ_s we must evaluate the operator $KW_s = iW_s^{-1}\nabla_s W_s$. To this end we must differentiate the operator U_s given in (11.24) This is not possible directly in the form in which this operator is given. However, it is easy to do so after this operator has been written in the ordered form

$$(11.26) \quad U_s = \exp - \tfrac{1}{2}(q_s^{+}-q_o^{+})(q_s^{-}-q_o^{-})\exp A^{+}(q_s^{-}-q_o^{-})\exp(q_o^{+}-q_s^{+})A^{-}$$

see [10]. Since now each exponent commutes with its derivative, differentiation with respect to s is possible.

We first find

$$iKU_s = -\frac{1}{2}\left[\nabla_s q_s^+ (q_s^- - q_o^-) + (q_s^+ - q_o^+)\nabla_s q_s^-\right]$$
$$+ \exp\left\{(q_s^+ - q_o^+)A^-\right\} A^+ \nabla_s q_s^- \exp\left\{(q_o^+ - q_s^+)A^-\right\} - \nabla_s q_s^+ A^-$$

Using the commutation rule

$$(11.27)\quad \exp\left\{p_1^+ A^-\right\} A^+ p_2^- \exp\left\{- p_1^+ A^-\right\} = A^+ p_2 + p_1^+ p_2^- \quad ,$$

see [8], we find

$$(11.28)\quad KW_s = i\left[(A^+ - q_o^+)\nabla q_s^- - \nabla_s q_s^+ (A^- - q_o^-)\right] + \eta_s - \nabla_s \theta_s \quad ,$$

when we use the abbreviation

$$(11.29)\quad \eta_s = -\frac{1}{2}\left[\nabla_s q_s^+ (q_s^- + q_o^-) - (q_s^+ + q_o^+)\nabla_s q_s^-\right] \quad .$$

We now should go over to an N_o-representation and determine the diagonal elements of the matrix which represents the operator KW_s . The N_o-representation of states $\underline{\Phi}$ is their representation in terms of functionals of the occupation number distributions $\nu(p)$. To determine the matrix elements we should take two eigenstates $\underline{\Phi}^{(1)}$, $\underline{\Phi}^{(2)}$ of N_o and form $(\underline{\Phi}^{(1)}, KW_s \underline{\Phi}^{(2)})$. The representers of these eigenstates would be functionals which vanish except if the functions $\nu(p)$ are equal to two particular functions $\nu_1(p)$ and $\nu_2(p)$ respectively. Clearly, the operators $A^{\pm}(p')$ transform such an eigenstate $\underline{\Phi}^{(1)}$ or $\underline{\Phi}^{(2)}$ into a

different -- orthogonal -- eigenstate associated with a function $\nu(p)$ differing from $\nu_1(p)$ or $\nu_2(p)$ in that $\nu(p')$ differs by ± 1 from $\nu_1(p')$ or $\nu_2(p')$. Clearly then, the matrix elements corresponding to the operators b^+A^- and A^+b^- are to be classed as off-diagonal elements.

The term $\eta_s - \nabla_s \theta_s$ occurring in (11.28), however, consisting in the multiplication by a plain number, is to be classed as a pure diagonal matrix. The condition that diagonal terms be absent, therefore, leads to the condition

$$\nabla_s \theta_s = \eta_s \quad , \tag{11.30}$$

from which θ_s can be determined

$$\begin{aligned} \theta_s = {} & \frac{i}{2} \int_0^s [q_\sigma^+ \nabla_\sigma q_\sigma^- - \nabla_\sigma q_\sigma^+ \cdot q_\sigma^-] d\sigma \\ & + \frac{i}{2} [q_\sigma^+ q_s^- - q_s^+ q_0^-] \quad . \end{aligned} \tag{11.31}$$

Because of the independence of the functional $h_s \{ \nu \}$ from s, cf. (11.20), we have

$$\int_0^s h_\sigma(N_0) d\sigma = sH_0 \quad . \tag{11.32}$$

The asymptotic formulas (3.3) and (3.5) therefore become

$$\begin{aligned} T_s(\tau) & \sim U_s \exp \{ i\theta_s \} \exp \{ -i\tau s H_0 \} \\ & = \exp \{ i\theta_s \} \exp \{ -i\tau s H_s \} U_s \quad . \end{aligned} \tag{11.33}$$

For $s = 1$, in particular, we have

$$(11.34)\quad T_s(\tau) \sim U_1 \exp\left\{ i\theta_1 \right\} \exp\left\{ -i\tau H_o \right\} = \exp\left\{ i\theta_1 \right\} \exp\left\{ -iH_1 \right\} U_1$$

with

$$(11.35)\quad U_1 = \exp\left\{ -A^+ q_o^- + q_o^+ A^- \right\} ,$$

and

$$(11.36)\quad \theta_1 = -\frac{i}{2} \int_o^1 [\nabla q_s^+ q_s^- - q_s^+ \nabla q_s^-] ds ,$$

because of (11.14), (11.16),

$$(11.37)\quad H_1 = A^+ h A^- .$$

Formula (11.34) gives the asymptotic description of the Schrödinger operator in the present case.

The validity of the asymptotic description (11.33) can easily be deduced from the exact expression for the Schrödinger operator $T_s(\tau)$. This exact expression can be written in different forms. For the present purpose the expression

$$(11.38)\quad T_s = \exp\left\{ i\rho_s \right\} \exp\left\{ (A^+ - q_o^+) r_s^- - r_s^+ (A^- - q_o^-) \right\} \exp\left\{ -i\tau s (A^+ - q_o^+) h (A^- - q_o^-) \right\}$$

is appropriate. In it

$$(11.39)\quad r_s^{\pm} = \mp\, i\tau h \int_0^s \exp\left\{ \pm\, i\tau(s-\sigma)h\,[q_\sigma^{\pm} - q_0^{\pm}]d\sigma \right.$$

and

$$(11.40)\quad \rho_s = \int_0^s \Big[\tfrac{1}{2}(q_\sigma^{+} - q_0^{+})hr_\sigma^{-} - \tfrac{1}{2}\, r_\sigma^{+}h(q_\sigma^{-} - q_0^{-})$$

$$- (q_\sigma^{+} - q_0^{+})h(q_\sigma^{-} - q_0^{-}) \Big]\, d\sigma \quad .$$

In order to verify that the expression (11.38) is the solution of equation (11.13) we first write it in the form

$$(11.41)\quad T_s = \exp\left\{ i\rho_s - \tfrac{1}{2}\, r_s^{+}\, r_s^{-} \right\} \exp\left\{ (A^{+} - q_0^{+})r_s^{-} \right\}$$

$$= \exp\left\{ r_s^{+}(q_0^{-} - A^{-}) \right\} \exp\left\{ -i\tau s(A^{+} - q_0^{+})h(A^{-} - q_0^{-}) \right\}$$

and then differentiate with respect to τ . Using the commutation rules for $\exp\left\{ A^{+}b^{-} - b^{-}A^{+} \right\}$, cf. [10], we find

$$i\left(\nabla_s T_s\right) T_s^{-1} = -\nabla_s \rho_s\ \tfrac{i}{2}(\nabla_s r_s^{+}\cdot r_s^{-} + r_s^{+}\nabla_s r^{-}) + i(A^{+} - q_0^{+})\nabla_s r_s^{-}$$

$$- i \exp\left\{ (A^{+} - q_0^{+})r_s^{-} \right\} \nabla_s r_s^{+}\cdot(A^{-} - q_0^{-}) \exp\left\{ (q_0^{+} - A^{+})r_s^{-} \right\}$$

$$+ \tau \exp\left\{ (A^{+} - q^{+})r_s^{-} \right\} \exp\left\{ r_s^{+}(q_0^{-} - A^{-}) \right\} (A^{+} - q_0^{+})h(A^{-} - q_0^{-})$$

$$\exp\left\{ r_s^{+}(A_s^{-} - q_0^{-}) \right\} \exp\left\{ (q_0^{+} - A^{+})r_s^{-} \right\}$$

$$= -\nabla_s \rho_s - \tfrac{i}{2}[(\nabla_s r_s^{+})r_s^{-}\ \nabla_s r_s^{-}\ ] + i(A^{+} - q_0^{+})\nabla_s r_s^{-} - i\left(\nabla_s r_s\right)(A^{-} - r_s^{-}\cdot$$

$$+ \tau(A^{+} - r_s^{+} - q_0^{+})h(A^{-} - r_s^{-} - q_0^{-}) = \tau(A^{+} - q_s^{+})h(A^{-} - q_s^{-}) = \tau H_s$$

as desired.

In order to determine the asymptotic expansion of the expression (11.38) we start with the expansion

$$r_s^{\pm} \sim q_s^{\pm} - q_s^{\pm} \mp i(\tau h)^{-1} \nabla_s q_s^{\pm} \tag{11.42}$$

whence

$$\nabla_s \rho_s \sim \frac{i}{2}[(q_s^{+} - q_o^{+}) \nabla_s q_s^{-} - \nabla_s q_s^{-} - (\nabla_s q_s^{+})(q_s^{-} - q_o^{-})] \tag{11.43}$$

$$= \eta_s = \nabla_s \theta_s$$

cf. (11.29), (11.30). Thus, as seen from (11.33), (11.24), formula (11.38) agrees asymptotically with formula (11.33).

Appendix

Remark I: Since our notation differs from that of Born and Fock, a remark may be added concerning the significance of a time dependent Hamiltonian. Although it would not be necessary to do so we shall interpret the operator $H(t) = H(t, \tau)$ with which we deal as the Hamiltonian energy operator of a physical object in the sense of quantum theory. In the Heisenberg picture of this theory, to every physical quantity an operator is assigned which depends on the time t. The dependence of the operator $H = H(t)$ on the time t should not, however, be confused with this time dependence. The operators $H(t)$ at different times correspond to different physical quantities, and the operators $H(t)$ are the operators which correspond to these different quantities in the Schrödinger picture. We may consider each of these quantities as a function of the basic operators of the object, such as momentum p and position q if the object is a single particle. - The operator $H(t)$ may then be expressed in the form

$$H(t) = H(t; p(t_o)\, q(t_o)) \quad .$$

Since the time dependence of these operators in the Heisenberg picture is induced by the time dependence of the operators p and q, our operator at the time $t = t'$ becomes $H(t;p(t'),q(t'))$. This operator can be expressed with the aid of the Schrödinger operator in terms of $H(t)$, namely

$$H(t;p(t'),q(t') = T^{-1}(t')H(t)T(t') \ .$$

Born and Fock denote the latter operator by $H(t')$ not showing explicitly its dependence on t; they denote our operator $H(t)$ by $H^{(o)}$.

Appendix (2)

Remark II: In terms of the kernels $(h,\alpha|F_1|h',\alpha')$ and $(h,\alpha|F_2|h',\alpha')$ of F_1 and F_2, identity (9.17) reads

$$\iint \delta_-(h-h'')(h,\alpha|F_1|h'',\alpha'')\delta_-(h''-h')(h'',\alpha''|F_2|h',\alpha')\,dm(\alpha'')\,dh''$$

$$= \delta_-(h-h')\iint \Big\{(h,\alpha|F_1|h'',\alpha'')\delta_-(h''-h')(h'',\alpha''|F_2|h',\alpha')$$

$$+ \delta_-(h-h'')(h,\alpha|F_1|h'',\alpha'')(h'',\alpha''|F_2|h',\alpha')\Big\}\,dm(\alpha'')\,dh''$$

and is thus seen to be equivalent with the identity

$$\delta_-(h-h'')\delta_-(h''-h') = \delta_-(h-h')[\delta_-(h''-h') + \delta_-(h-h'')] \;;$$

which follows from the identity

$$\frac{1}{z}\,\frac{1}{z''} = \frac{1}{z+z''}\left[\frac{1}{z''} + \frac{1}{z}\right]$$

by letting z and z'' approach the real values $h-h''$ and $h''-h'$ through complex values with positive imaginary parts.

Bibliography

[1] Born, M., Das Adiabatenprinzip in der Quantenmechanik, Zeitschrift fuer Physik, Vol. 40, pp. 167-192, 1926.

[2] Born, M., and Fock, V., Beweis des Adiabatensatzes, Zeitschrift fuer Physik, Vol. 51, pp. 165-180, 1928.

[3] Güttinger, P., Das Verhalten von Atomen im magnetischen Drehfeld. Zeitschrift, fuer Physik, Vol. 73, pp. 169-184. Nov. 1931 - Jan. 1932.

[4] Friedrichs, K. O., Ueber die Spektralzerlegung eines Integraloperators, Mathematische Annalen, Vol. 115, No. 2, pp. 249-272, 1938.

[5] Møller, C., General Properties of the Characteristic Matrix in the Theory of Elementary Particles, Det Kgl. Danske Videnskabernes Selskab, matemtisk-fysiske Meddelelser, Vol. 22, No. 1, 1945 and No. 9, 1946.

[6] Friedrichs, K. O., On the Perturbation of Continuous Spectra, Communications on Pure and Applied Mathematics, Vol. 1, No. 4, pp. 361-406, December 1948.

[7] Kato, T., On the Adiabatic Theorem of Quantum Mechanics, Journal of the Physical Society of Japan, Vol. 5, pp. 435-439, Nov.-Dec. 1950.

[8] Keller, H. and Keller, J., On Systems of Linear Ordinary Lifferential Equations, Geophysical Research Directorate, Research Report No. EM-33, July 1951.

[9] Snyder, H. S., Remarks Concerning the Adiabatic Theorem and the S-Matrix, Physical Review, Vol. 83, pp. 1154-1159,1951.

[10] Friedrichs, K.O., Mathematical Aspects of the Quantum Theory of Fields, Part III, Section 16, and Part IV. Communications on Pure and Applied Mathematics, Vol. 5, No. 1, February 1952, Vol. V, No. 4, November 1952, or book with same title.

[11] Kato, T., Integration of the Equation of Evolution in a Banach Space, Journal of the Mathematical Society of Japan, Vol. 5, pp. 208-234, 1953.

[12] Wasow, W., Introduction to the Asymptotic Theory of Ordinary Linear Differential Equations, U. S. Department of Commerce, National Bureau of Standards, Report No. 54-6, 1953.

[13] Moses, H. E., Properties of the Scattering Operator in Quantum Mechanics, Part I: The Properties of the Scattering Operator for the Time-Dependent Schrödinger Equation, Research Report CX 12, October 1953. Part II: The Scattering Operator Formalism and Other Formalisms, Research Report CX 13, December 1953.

Application of Variational Principles to Scattering Problems, Physical Review, Vol. 96, No. 2, pp. 519-522, 1954.

The Scattering Operator and the Adiabatic Theorem, Il Nuovo Cimento, Vol. 1, pp. 103-131, 1955.

OFFICE OF ORDNANCE RESEARCH

DISTRIBUTION LIST

FOR

TECHNICAL REPORTS

Office of Ordnance Research
Box CH, Duke Station
Durham, North Carolina (10)

Office, Chief of Ordnance
Washington 25, D. C.
Attn: ORDTB-PS (1)

Commanding General
White Sands Proving Ground
Las Cruces, New Mexico (1)

Office of Naval Research
Washington 25, D. C.
Attn: Mathematics Branch (1)

Commanding General
Aberdeen Proving Ground, Maryland
Attn: BRL (2)

Commanding General
Redstone Arsenal
Huntsville, Alabama (1)

Commanding Officer
Rock Island Arsenal
Rock Island, Illinois (1)

Commanding General
Research and Engineering Command
Army Chemical Center, Maryland (1)

Chief, Ordnance Development Div.
National Bureau of Standards
Washington 25, D. C. (1)

Commanding Officer
Watertown Arsenal
Watertown 72, Mass. (1)

Technical Reports Library
SCEL, Evans Signal Corps Lab.
Belmar, New Jersey (1)

Jet Propulsion Laboratory
California Institute of Technology
4800 Oak Grove Drive
Pasadena 3, California (1)

Commanding Officer
Engineering Res. + Dev. Labs.
Fort Belvoir, Virginia (1)

Commander
U.S. Naval Proving Ground
Dahlgren, Virginia (1)

Chief, Bureau of Ordnance (AD3)
Department of the Navy
Washington 25, D. C. (1)

U.S. Naval Ordnance Laboratory
White Oak, Silver Spring 19, Md.
Attn: Library Division (1)

Director
National Bureau of Standards
Washington 25, D. C. (1)

Corona Laboratories
National Bureau of Standards
Corona, California (1)

Commanding Officer
Frankford Arsenal
Bridesburg Station
Philadelphia 37, Penna. (1)

Technical Information Service
P.O. Box 62
Oak Ridge, Tennessee
Attn: Reference Branch (1)

Commanding Officer
Signal Corps Engineering Lab.
Fort Monmouth, New Jersey
Attn: Director of Research (1)

The Director
Naval Research Laboratory
Washington 25, D. C.
Attn: Code 2021 (1)

Chief, New York Ordnance District
180 Varick Street
New York 14, N. Y. (2)

DISTRIBUTION LIST (CONT.)

Director, Applied Physics Lab.
Johns Hopkins University
8621 Georgia Avenue
Silver Spring 19, Maryland (1)

Commanding General
Air University
Maxwell Air Force Base, Alabama
Attn: Air University Library (1)

Canadian Joint Staff
1700 Massachusetts Ave. N.W.
Washington 6, D. C.
THRU: ORDGU-SE (1)

Commanding General
Air Res. + Dev. Command
P.O. Box 1395
Baltimore 3, Maryland
Attn: RDD (1)

Commanding General
Air Res. + Dev. Command
P.O. Box 1395
Baltimore 3, Maryland
Attn: RDR (1)

Armed Services Tech. Info. Agency
Document Service Center
Knott Building
Dayton 2, Ohio
Attn: DSC-SD (5)

Commander
U.S. Naval Ord. Test Station,
Inyokern
China Lake, California
Attn: Technical Library (1)

U.S. Atomic Energy Commission
Document Library
19th + Constitution Ave.
Washington 25, D. C. (1)

Commanding General
Air Material Command
Wright-Patterson Air Force Base
Dayton 2, Ohio
Attn: F. N. Budd, Chief Scientist
Flight Research Lab. (1)

Office of the Chief Signal Officer
Engineering + Technical Division
Engineering Control Branch
Room 28273, Pentagon Building
Washington 25, D. C.
Attn: SIGGD (1)

NAC for Aeronautics
1724 F Street, N. W.
Washington 25, D. C.
Attn: Mr. E. B. Jackson, Chief
Officer of Aeronautical
Intelligence (1)

Scientific Information Section
Research Branch
Research + Development Division
Office, Assistant Chief of Staff,
G-4
Department of the Army
Washington 25, D. C. (1)

Samuel Feltman Labs.
Picatinny Arsenal
Dover, New Jersey (1)

Commanding Officer
U. S. Naval Factory
Indian Head, Maryland (1)

Dr. B. H. Bissinger
Department of Mathematics
Lebanon Valley College
Annville, Pa. (1)

Date Due

DEC 6 '55
NOV 11 60
~~NOV 28 60~~
FEB 10 '61
MAY 2 '62
2-2.65 ILL
Brookhaven Natl Lab
MAY 28 '65
7/19/66 ILL
Univ of Wisconsin
4/26/67 ILL Univ of Toronto
MAY 30 1969
AUG 13 1969
JAN 30 1988
FEB 10 1997

PRINTED IN U.S.A.

NYU-IMM-218 c.1

Friedrichs
AUTHOR

On the adiabatic theo-
TITLE

rem in quantum theory.

NYU-IMM-218

Friedrichs.

On the adiabatic theorem
in quantum theory. Part I.

~~NEW YORK UNIVERSITY~~
~~INSTITUTE OF MATHEMATICAL SCIENCES~~
~~LIBRARY~~
~~25 Waverly Place, New York 3, N.Y.~~

NEW YORK UNIVERSITY
COURANT INSTITUTE - LIBRARY
251 Mercer St. New York, N.Y. 10012